

Conformational analysis of 1,3,2-dioxaphospholan-yl and 4,5-benzo-1,3,2-dioxaphosphol-2-yl 2,2,2-trifluoroacetate

Ishmaeva E., Vereshchagina Y., Chachkov D., Alimova A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Conformational analysis of 1,3,2-dioxaphospholan-2-yl 2,2,2-trifluoroacetate and 4,5-benz-1,3,2-dioxaphosphol-2-yl 2,2,2-trifluoroacetate was carried out using the method of dipole moments and quantumchemical calculations (DFT B3LYP/6-31G*). Both compounds are found to exist as an axial conformer with preferably syn arrangement of the carbonyl group and the lone electron pair. © 2012 Pleiades Publishing, Ltd.

<http://dx.doi.org/10.1134/S1070363212110059>
